

Numerical Analysis - Approximating Functions

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Notation: Equation numbers are placed in parentheses, (**Eq. 1**), at the end of the sentence preceding the mathematical presentation of the equation. They should not be read as if they are part of the sentence. When reference is made to an equation, the word "equation" will be spelled out and not abbreviated. Mathematical symbols are not in all cases precise. Greek symbols will show as such on a Windows operating system, but not a Unix or Mac system.

Series Approximation

Given values of a function $f(x)$ at a finite number of discrete points (n),

$$\begin{array}{ccccccc} x_0, & x_1, & x_2, & x_3, & \dots, & x_{n-1}, & x_n \\ f(x_0), & f(x_1), & f(x_2), & f(x_3), & \dots, & f(x_{n-1}), & f(x_n) \end{array}$$

the goal is to construct an arbitrary, but simpler, function $p(x)$ in the form of series that takes on the values of f_i at the n points x_i , that is (**Eq. 1**),

$$\begin{aligned} p(x) &\equiv f(x), \text{ for } x_0 < x < x_n \\ &\text{and possibly for } x < x_0 \text{ or } x > x_n \end{aligned}$$

that is to say (**Eq. 2**)

$$p(x) = f(x_i), \text{ for } x_0, \dots, x_n$$

The function $p(x)$ can take a variety of forms, such as

- when $p(x)$ is a polynomial, the process of representing $f(x)$ by $p(x)$ is called a **polynomial approximation**,
- when $p(x)$ is a finite trigonometric series, the process of representing $f(x)$ by $p(x)$ is called a **trigonometric approximation**, and
- in like manner $p(x)$ may be a series of:
 - exponential functions
 - Legendre polynomials
 - Bessel functions
 - etc.

Approximating functions are the basis for interpolation schemes, and interpolation schemes are the basis for numerical quadrature relations. Thus approximating functions represent an important element in numerical methods.

Difference Tables

Before we consider polynomial interpolation schemes, we should develop the concept of difference tables in the following document called [Difference Tables](#).

Interpolation

Now that we have the concept of differences and their notation, we can develop the most elementary interpolation schemes known as polynomial interpolation found in the following document [Polynomial Interpolation](#).

A frequently encounter interpolation problem is one in which the data is not equally spaced in the independent variable. This leads us to consider the material in the following document on [Non-Equidistant Interpolation](#).

Least Square Data Analysis

Finally, we should explore a different approach to approximating functions known as least squares as discussed in the following document [Least Squares](#).

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PHYS 251 - Introduction to Computer Techniques in Physics**Difference Tables**

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Notation: Equation numbers are placed in parentheses, (Eq. 1), at the end of the sentence preceding the mathematical presentation of the equation. They should not be read as if they are part of the sentence. When reference is made to an equation, the word "equation" will be spelled out and not abbreviated. Mathematical symbols are not in all cases precise. Greek symbols will show as such on a Windows operating system, but not a Unix or Mac system.

Horizontal Difference Table

Difference tables lend themselves to the use of spreadsheets as a means of solving many problems rather than resorting to writing computer code in either Fortran or C/C++. One type of difference table is known as a **horizontal difference table** in which differences are maintained on horizontal rows with the function as shown below for which successive differences through the fourth are denoted by $\Delta_1 f_i(x)$, $\Delta_2 f_i(x)$, $\Delta_3 f_i(x)$, and $\Delta_4 f_i(x)$.

x_i	$f_i(x)$	$\Delta_1 f_i(x)$	$\Delta_2 f_i(x)$	$\Delta_3 f_i(x)$	$\Delta_4 f_i(x)$
...
x_{-2}	f_{-2}	$f_{-2} - f_{-3}$	$f_{-2} - 2f_{-3} + f_{-4}$
x_{-1}	f_{-1}	$f_{-1} - f_{-2}$	$f_{-1} - 2f_{-2} + f_{-3}$	$f_{-1} - 3f_{-2} + 3f_{-3} - f_{-4}$...
x_0	f_0	$f_0 - f_{-1}$	$f_0 - 2f_{-1} + f_{-2}$	$f_0 - 3f_{-1} + 3f_{-2} - f_{-3}$	$f_0 - 4f_{-1} + 6f_{-2} - 4f_{-3} + f_{-4}$
x_1	f_1	$f_1 - f_0$	$f_1 - 2f_0 + f_{-1}$	$f_1 - 3f_0 + 3f_{-1} - f_{-2}$	$f_1 - 4f_0 + 6f_{-1} - 4f_{-2} + f_{-3}$
x_2	f_2	$f_2 - f_1$	$f_2 - 2f_1 + f_0$	$f_2 - 3f_1 + 3f_0 - f_{-1}$	$f_2 - 4f_1 + 6f_0 - 4f_{-1} + f_{-2}$
x_3	f_3	$f_3 - f_2$	$f_3 - 2f_2 + f_1$	$f_3 - 3f_2 + 3f_1 - f_0$	$f_3 - 4f_2 + 6f_1 - 4f_0 + f_{-1}$
x_4	f_4	$f_4 - f_3$	$f_4 - 2f_3 + f_2$	$f_4 - 3f_3 + 3f_2 - f_1$	$f_4 - 4f_3 + 6f_2 - 4f_1 + f_0$
...

Error Propagation in Difference Tables

Errors propagate in a horizontal difference table as shown below, where ϵ is a small increment in the function f .

x_i	$f_i(x)$	$\Delta_1 f_i(x)$	$\Delta_2 f_i(x)$	$\Delta_3 f_i(x)$	$\Delta_4 f_i(x)$
...
x_{-2}	f_{-2}
x_{-1}	f_{-1}
x_0	$f_0(x) + \epsilon$	$\Delta_1 f_0(x) + \epsilon$	$\Delta_2 f_0(x) + \epsilon$	$\Delta_3 f_0(x) + \epsilon$	$\Delta_4 f_0(x) + \epsilon$
x_1	f_1	$\Delta_1 f_1(x) - \epsilon$	$\Delta_2 f_1(x) - 2\epsilon$	$\Delta_3 f_1(x) - 3\epsilon$	$\Delta_4 f_1(x) - 4\epsilon$
x_2	f_2	...	$\Delta_2 f_2(x) + \epsilon$	$\Delta_3 f_2(x) + 3\epsilon$	$\Delta_4 f_2(x) + 6\epsilon$
x_3	f_3	$\Delta_3 f_3(x) - \epsilon$	$\Delta_4 f_3(x) - 4\epsilon$
x_4	f_4	$\Delta_4 f_4(x) + \epsilon$
...

There are several points one should note about the propagation of the error.

1. The error moves to successive rows with successive differences.
2. The coefficients of ϵ 's are binomial coefficients with alternating signs.
3. The algebraic sum of the ϵ 's in any difference column is zero.
4. The first erroneous difference of any order is on the same horizontal line as the erroneous functional value.

Polynomial Interpolation

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Polynomial Interpolation

The justification for approximating with polynomials rest on a theorem by Weierstrass in 1885, to which

"...every continuous function in an interval (a,b) can be represented in that interval to any desired accuracy by a polynomial."

One can also show that the following propositions are true for a polynomial

1. nth differences of an nth-degree polynomial are constant for an arithmetic progression (equal interval) of the independent variable,
 2. if nth differences of a tabulated function for equal interval data are constant, the unknown function is a polynomial of degree n.
-

Example

Let $f(x) = x^2 + 3x + 2$. Forming differences in a horizontal difference table, we have the table shown below.

x_i	$f_i(x)$	$\Delta_1 f_i(x)$	$\Delta_2 f_i(x)$	$\Delta_3 f_i(x)$	$\Delta_4 f_i(x)$
0.000000	2.000000				
1.000000	6.000000	4.000000			
2.000000	12.000000	6.000000	2.000000		
3.000000	20.000000	8.000000	2.000000	0.000000	
4.000000	30.000000	10.000000	2.000000	0.000000	
5.000000	42.000000	12.000000	2.000000	0.000000	
6.000000	56.000000	14.000000	2.000000	0.000000	

Since the function is indeed a 2nd degree polynomial the 2nd differences are constant.

Polynomial Interpolation Retaining Second Differences

If we restrict our consideration to the retention of second differences and ignore all higher-order differences, there are four useful polynomial approximations that can be derived for equal-interval interpolation.

Newton's Forward Interpolation: Given values of a function $f(x)$ at a finite number of discrete points (n),

$$x_0, \quad x_1, \quad x_2, \quad x_3, \quad \dots, \quad x_{n-1}, \quad x_n$$

$$f(x_0) = f_0, \quad f(x_1) = f_1, \quad f(x_2) = f_2, \quad f(x_3) = f_3, \quad \dots, \quad f(x_{n-1}) = f_{n-1}, \quad f(x_n) = f_n$$

and letting $u = [(x - x_i) / (x_{i+1} - x_i)]$, then Newton's forward interpolation formula can be expressed using difference notation as

$$p(x) = p(x_0 + u\Delta x)$$

or substituting the difference values of the function, we have

$$p(x) = f_0 + u\Delta_1 f_1 + [u(u-1)/2!] \Delta_2 f_2 + [u(u-1)(u-2)/3!] \Delta_3 f_3 + \dots + [u(u-1)(u-2)\dots(u-n+1)/n!] \Delta_n f_n + \dots$$

which can be simplified by retaining only second order differences and substituting the functional values for the differences (Eq. 1)

$$p(x) = f_0 + u(f_1 - f_0) + [u(u-1)/2](f_2 - 2f_1 + f_0)$$

Since Newton's forward interpolation formula uses values of the function at points ahead in

the table, it can be used at the beginning of the tabulated values, but not at the end.

Newton's Backward Interpolation: Given values of a function $f(x)$ at a finite number of discrete points (n), and letting $u = [(x - x_i) / (x_i - x_{i-1})]$, then Newton's backward interpolation formula can be expressed using difference notation as

$$p(x) = p(x_0 + u\Delta x)$$

or substituting the difference values of the function, we have

$$\begin{aligned} p(x) = f_n + u\Delta_1 f_n + [u(u+1)/2!] \Delta_2 f_n + [u(u+1)(u+2)/3!] \Delta_3 f_n + \dots + \\ [u(u+1)(u+2)\dots(u+n-1)/n!] \Delta_n f_n + \dots \end{aligned}$$

which can be simplified by retaining only second order differences and substituting the functional values for the differences (Eq. 2)

$$p(x) = f_0 + u(f_0 - f_{-1}) + [u(u+1)/2](f_0 - 2f_{-1} + f_{-2})$$

which is useful for interpolating near the end of the tabulated functions.

Stirling's Central-Difference Interpolation: This interpolation formula is based on a diagonal difference table rather than a horizontal difference table. Without going into the distinctions between the two types of difference tables, we can write down an interpolation formula including only second differences that is similar to Newton's interpolation formulas. Thus given values of a function $f(x)$ at a finite number of discrete points (n), and letting $u = [(x - x_i) / (x_{i+1} - x_i)]$, Stirling's central-difference interpolation formula can be expressed using functional values as (Eq. 3)

$$p(x) = f_0 + (u/2)(f_1 - f_{-1}) + [u^2/2](f_1 - 2f_0 + f_{-1})$$

which also uses three successive points to approximate the function as does Newton.

Bessel's Central-Difference Interpolation: This interpolation formula is also based on a diagonal difference table rather than a horizontal difference table. We shall also write down an interpolation formula including only second differences that is similar to Newton's and Stirling's interpolation formulas. Thus given values of a function $f(x)$ at a finite number of discrete points (n), and letting $u = [(x - x_i) / (x_{i+1} - x_i)]$, Bessel's central-difference interpolation formula can be expressed using functional values as (Eq. 4)

$$p(x) = f_0 + u(f_1 - f_0) + [u(u-1)/4](f_2 - f_1 - f_0 + f_{-1})$$

which uses four successive points rather than three to approximate the function. Note that in equations 1, 2, 3, and 4, there is a zero-order term, a first-order term, and a second-order term. The zero- and first-order terms constitute essential a linear interpolation, while the second-order term is a correction term to that linear interpolation.

Example

Find $f(x) = \exp(-x)$, at the point $x = 1.7565$, given the following values of the function.

i	x_i	f_i
-2	1.730000000	0.177284100
-1	1.740000000	0.175520401
0	1.750000000	0.173773944
1	1.760000000	0.172044864
2	1.770000000	0.170332989

Forming the value of u for the four equidistance interpolation formulas, we have for Newton's forward, Stirling's, and Bessel's interpolation formulas

$$u = (x - x_0) / (x_1 - x_0) = (1.7565 - 1.75) / (1.76 - 1.75) = 0.0065 / 0.01 = + 0.65 ,$$

Newton's Forward Interpolation:

$$u(u - 1) / 2 = 0.65(0.65 - 1) / 2 = -0.11375 ,$$

Stirling's Central-Difference Interpolation:

$$u / 2 = 0.65 / 2 = 0.325 ,$$

$$u^2 / 2 = (0.65)^2 / 2 = 0.21125 ,$$

Bessel's Central-Difference Interpolation:

$$u(u - 1) / 4 = 0.65(0.65 - 1) / 4 = -0.056875 .$$

For Newton's backward formula, the value of u is given by

$$u = (x - x_1) / (x_1 - x_0) = (1.7565 - 1.76) / (1.76 - 1.75) = -0.0035 / 0.01 = -0.35 ,$$

Newton's Backward Interpolation:

$$u(u + 1) / 2 = -0.35(-0.35 + 1) / 2 = -0.11375 .$$

The following table evaluates the three terms that appear in each of the four interpolation formula. Note that in order to apply Newton's backward formula, we must re-label the points so that $i = -1, 0, 1$ become $i = -2, -1, 0$.

Interpolation Formula	Zero-Order Term	First-Order Term	Second-Order Term	$f(u)$
Newton's Forward	0.173773944	-0.001123902	-0.000001957	0.172648085
Newton's Backward	0.172044864	+0.000605178	-0.000001977	0.172648065
Stirling's Formula	0.173773944	-0.001129550	+0.000003671	0.172648065
Bessel's Formula	0.173773944	-0.001123902	-0.000001967	0.172648075
Exact Solution				0.172648076

It is evident that Bessel's interpolation formula has given us the most accurate result. This is in part true because Bessel's formula is known to be more accurate when u lies between 0.25 and 0.75.

Non-Equidistant Interpolation

A frequently encountered interpolation problem is one in which the data is not equally spaced in the independent variable. This leads us to consider Lagrangian interpolation in the following document on [Non-Equidistant Interpolation](#).

Non-Equidistant Interpolation

Lagrange's Formula

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Non-Equidistant Data Interpolation

The previous discussion of interpolation is predicated on equidistant intervals in the independent variable x . Sometimes it is inconvenient or impossible to obtain function values on an equidistant interval. In such cases, Lagrange's formula can be fashioned to only utilize such data as may be available.

The general form of Lagrange's interpolation formula is given by (Eq. 1)

$$p(x) = \sum_{j=0}^n \left\{ \left[\prod_{i=0, i \neq j}^n (x - x_i) \right] / \left[(x - x_j) \prod_{i=0, i \neq j}^n (x_j - x_i) \right] \right\}$$

where

$$\prod_{i=0}^n (x - x_i) = (x - x_1)(x - x_2)\dots(x - x_n)$$

$$\prod_{i=0, i \neq j}^n (x_j - x_i) = (x_j - x_0)(x_j - x_{i-1})(x_j - x_{i+1})\dots(x_j - x_n)$$

We should note that

1. lagrange's formula does not involve successive differences as does Newton's, Stirling's and Bessel's interpolation formulas.
2. Lagrange's formula does involve $n+1$ successive pairs of variables (x_n, f_n) .
3. Although Lagrange's formula works for non-equidistant data, it is not restricted to such a limitation, i.e., it can be applied to equidistant data.
4. If we know rates of change (differences) or rates of rates of change of the function, their neglect is to ignore information.

Cubic Lagrangian Interpolation

Suppose one wishes to construct a cubic polynomial through four successive points of a

data set which we will label as $(x_1, f_1), (x_2, f_2), (x_3, f_3)$, and (x_4, f_4) . This can be accomplished from our general relation for $n+1$ points where we can construct the following relation (Eq. 2)

$$p(x) = l_{1,4} f_1 + l_{2,4} f_2 + l_{3,4} f_3 + l_{4,4} f_4$$

where

$$l_{1,4} = [(x - x_2)(x - x_3)(x - x_4)] / [(x_1 - x_2)(x_1 - x_3)(x_1 - x_4)]$$

$$l_{2,4} = [(x - x_1)(x - x_3)(x - x_4)] / [(x_2 - x_1)(x_2 - x_3)(x_2 - x_4)]$$

$$l_{3,4} = [(x - x_1)(x - x_2)(x - x_4)] / [(x_3 - x_1)(x_3 - x_2)(x_3 - x_4)]$$

$$l_{4,4} = [(x - x_1)(x - x_2)(x - x_3)] / [(x_4 - x_1)(x_4 - x_2)(x_4 - x_3)]$$

If one wishes, this expression can be written in the form (with a little algebra) as

$$p(x) = ax^3 + bx^2 + cx + d$$

However, from the computational point of view there is no real advantage in doing so.

Example

Find the cubic polynomial whose graph contains the four successive points $(0,1), (1,2), (2,0)$, and $(3,-2)$. Setting $x_1 = 0, f_1 = 1, x_2 = 1, f_2 = 2, x_3 = 2, f_3 = 0$, and $x_4 = 3, f_4 = -2$, we can form the values of the l s

$$\begin{aligned} l_{1,4} &= [(x - x_2)(x - x_3)(x - x_4)] / [(x_1 - x_2)(x_1 - x_3)(x_1 - x_4)] \\ &= [(x - 1)(x - 2)(x - 3)] / [(0 - 1)(0 - 2)(0 - 3)] \\ &= [(x - 1)(x - 2)(x - 3)] / -6 \end{aligned}$$

$$\begin{aligned} l_{2,4} &= [(x - x_1)(x - x_3)(x - x_4)] / [(x_2 - x_1)(x_2 - x_3)(x_2 - x_4)] \\ &= [(x - 0)(x - 2)(x - 3)] / [(1 - 0)(1 - 2)(1 - 3)] \\ &= [x(x - 2)(x - 3)] / 2 \end{aligned}$$

$$\begin{aligned} l_{3,4} &= [(x - x_1)(x - x_2)(x - x_4)] / [(x_3 - x_1)(x_3 - x_2)(x_3 - x_4)] \\ &= [(x - 0)(x - 1)(x - 3)] / [(2 - 0)(2 - 1)(2 - 3)] \\ &= [x(x - 1)(x - 3)] / -2 \end{aligned}$$

$$\begin{aligned} l_{4,4} &= [(x - x_1)(x - x_2)(x - x_3)] / [(x_4 - x_1)(x_4 - x_2)(x_4 - x_3)] \\ &= [(x - 0)(x - 1)(x - 2)] / [(3 - 0)(3 - 1)(3 - 2)] \\ &= [x(x - 1)(x - 2)] / 6. \end{aligned}$$

Inserting the values for the l s into Equation 2, we have

$$\begin{aligned} f(x) &= l_{1,4} f_1 + l_{2,4} f_2 + l_{3,4} f_3 + l_{4,4} f_4 \\ &= \{[(x - 1)(x - 2)(x - 3)] / -6\} 1 + \{[x(x - 2)(x - 3)] / 2\} 2 + \{[x(x - 1)(x - 3)] / -2\} 0 - \{[x(x - 1)(x - 2)] / 6\} (-2) \end{aligned}$$

$$= \left(-\frac{1}{6}\right) [(x - 1)(x - 2)(x - 3)] + [x(x - 2)(x - 3)] + \left(-\frac{1}{3}\right) [x(x - 1)(x - 2)].$$

Multiplying out the terms and collecting yields the desired polynomial

$$f(x) = \frac{1}{2}x^3 - 3x^2 + \frac{7}{2}x + 1.$$

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PHYS 251 - Introduction to Computer Techniques in Physics

Least Squares

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Defining a "Close Fitting" Approximating Function

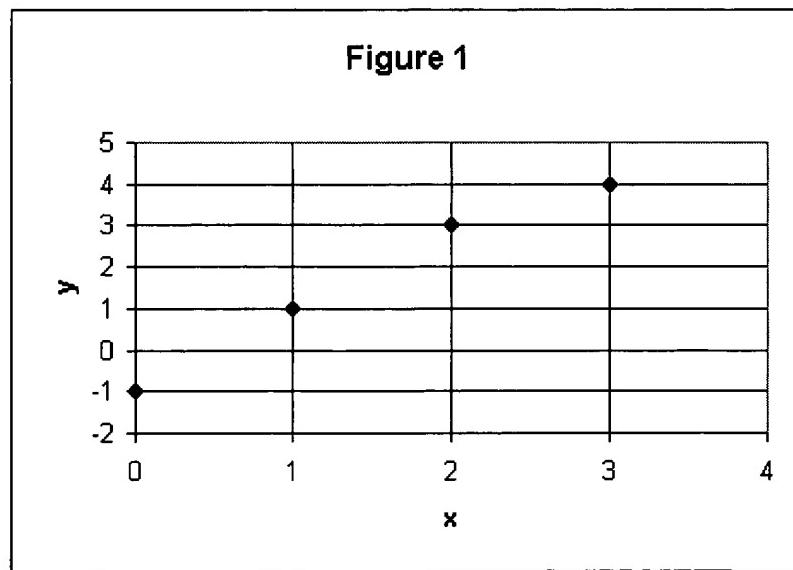
Earlier we had discussed approximating functions ([Approximating Functions](#)). In that discussion the approximating function contained all of the points of a given discrete function, i.e., the function was constructed such that it agreed precisely with the discrete points used in its construction. Suppose now we wish to construct approximating functions whose graphs need not necessarily contain the points of given discrete function, but which "fits the function closely." Such is the method known as least squares.

In order to understand this idea of "fits the function closely," let us consider a simple example. Given the points (0, -1), (1, 1), (2, 3), and (3, 4), let us find the straight line $f(x) = a_1 + a_2 x$, which in some sense "fits the data closely."

Figure 1 shows a graph of the four points that we wish to fit. One means of determining what is a close fit, is to minimize the vertical distances between the given points and the constructed line. Let us calculate the "errors" or "how far the line misses the given points" as follows (**Eq. 1**)

$$\varepsilon_1 = a_1 + a_2 x_1 - f_1 ,$$

$$\varepsilon_2 = a_1 + a_2 x_2 - f_2 ,$$



$$\varepsilon_3 = a_1 + a_2 x_3 - f_3 ,$$

$$\varepsilon_4 = a_1 + a_2 x_4 - f_4 .$$

where our object is to minimize the total error. We could do that by considering the total error E. Let us first consider just the sum of the individual errors as given by (**Eq. 2**)

However, a simple sum will not suffice as the following example illustrates. Suppose the values of the errors are as shown

$$E = (0.1) + (-0.1) + (0.2) + (-0.2) = 0 .$$

Although the sum gives us a minimum, it is meaningless since clearly the total error is not zero. Another possible means of minimizing is to take the absolute values of the errors, but this means that the function E is not always differentiable. To preserve the differentiability of E and yet avoid the sign problem, we can minimize the squares of the errors as in (Eq. 3)

$$E = \varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2 + \varepsilon_4^2 .$$

Equation 3 is the desirable definition of E since (i) it is always differentiable, (ii) individual terms are non-negative, and (iii) because of the parabolic structure E always has a unique minimum.

Minimizing the Total Error

Let us construct our total error function for the given example (Eq. 4)

$$E = [a_1 + 1]^2 + [(a_1 + a_2) - 1]^2 + [(a_1 + 2a_2) - 3]^2 + [(a_1 + 3a_2) - 4]^2 .$$

In order to minimize, we want to set the partial derivative of E with respect to each of the parameters in the linear fit, a_1 and a_2 , as shown (Eq. 5)

$$\delta E / \delta a_1 = 0 , \delta E / \delta a_2 = 0 .$$

which yields the two linear algebraic equations

$$\begin{aligned} 4 a_1 + 6 a_2 &= 7 , \\ 6 a_1 + 14 a_2 &= 19 , \end{aligned}$$

whose solution is

$$\begin{aligned} a_1 &= -0.8 , \\ a_2 &= 1.7 . \end{aligned}$$

Thus the approximating function that "fits the data closely" is (**Eq. 6**)

$$f(x) = a_1 + a_2 x = -0.8 + 1.7 x,$$

and the sense in which it fits closely is that it minimizes the squares of the vertical distances between the approximating function and the discrete points.

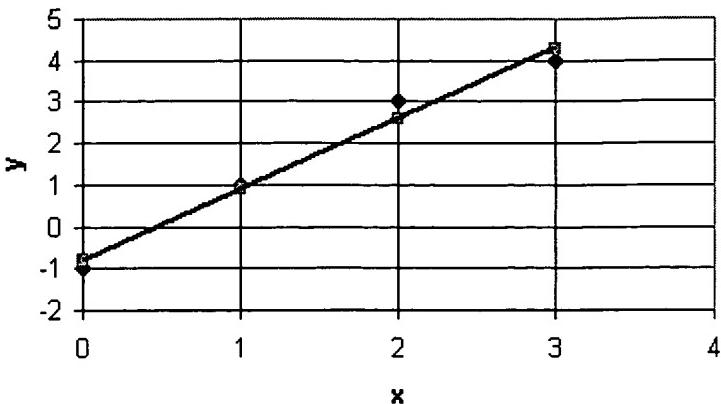
Figure 2

Figure 2 shows a graph of the four points that we wish to fit along with approximating function that minimizes the squares of the vertical distances between the given points and the constructed line.

Are there other ways to define "fits closely?" Yes, for example, minimize the squares of the perpendicular distances rather than the vertical distances. However, this is a considerably harder problem to solve. Therefore, we will restrict ourselves to the standard definition of the least squares technique and minimize the vertical distances.

Periodic or Quasi-Periodic Approximating Functions in Least Squares.

Let us consider a second example, which reveals more of the subtle aspects of the method of least squares.

The general description of the method of least squares is as follows. Given the set of discrete points $(x_1, f_1), (x_2, f_2), (x_3, f_3), \dots (x_n, f_n)$, let $g(x)$ be a continuous function chosen such as to minimize the squares of the vertical distances, that is, minimize the total error E (**Eq. 7**)

$$E = [g(x_1) - f_1]^2 + [g(x_2) - f_2]^2 + [g(x_3) - f_3]^2 + \dots + [g(x_n) - f_n]^2.$$

assuming that $g(x)$ contains m independent parameters a_1, a_2, \dots, a_m . In order to minimize E with respect to each of the m independent parameters, we solve the system of algebraic equations given by (**Eq. 8**)

$$\delta E / \delta a_1 = 0, \delta E / \delta a_2 = 0, \delta E / \delta a_3 = 0, \dots, \delta E / \delta a_m = 0.$$

to yield the desired values of the m independent parameters a_1, a_2, \dots, a_m .

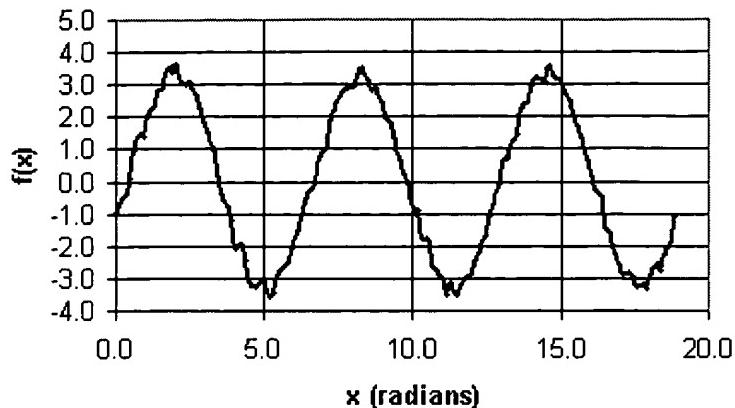
Now let us consider the oscilloscope trace shown in Figure 3. For our oscilloscope trace, what is the functional form for $g(x)$ that "fits closely" the data? Some possibilities are (Eq. 9)

$$\text{linear: } g(x) = a_1 + a_2 x,$$

$$\text{quadratic: } g(x) = a_1 + a_2 x + a_3 x^2,$$

$$\text{cubic: } g(x) = a_1 + a_2 x + a_3 x^2 + a_4 x^3.$$

Figure 3



However, the choice of the approximating function $g(x)$ to be used must depend on some knowledge of the behavior of the phenomenon under observation. For the oscilloscope trace in Figure 3, the behavior is clearly periodic and a function like (Eq. 10)

$$g(x) = a_1 \sin(x) + a_2 \cos(x).$$

would be a reasonable place to begin. Let us assume that the five points $(0, -0.9)$, $(\pi/4, 1.5)$, $(\pi/2, 3.1)$, $(3\pi/4, 3.0)$, and $(\pi, 1.1)$ are on the graph in Figure 3, so that the total error is

$$E = [a_1 \sin(0) + a_2 \cos(0) + 0.9]^2 + [a_1 \sin(\pi/4) + a_2 \cos(\pi/4) - 1.5]^2 + [a_1 \sin(\pi/2) + a_2 \cos(\pi/2) - 3.1]^2 + [a_1 \sin(3\pi/4) + a_2 \cos(3\pi/4) - 3.0]^2 + [a_1 \sin(\pi) + a_2 \cos(\pi) - 1.1]^2.$$

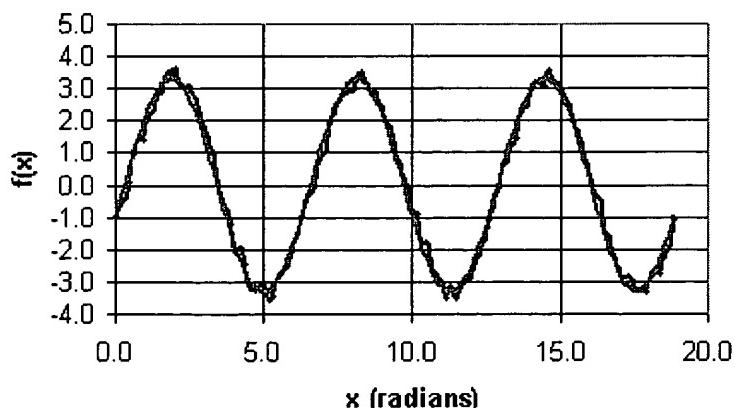
Next minimizing with respect to the two independent parameters a_1 and a_2 yields two algebraic expressions that can immediately be solved for a_1 and a_2 or

$$a_1 = 3.14 \text{ and } a_2 = -1.02,$$

so that (Eq. 11)

$$g(x) = 3.14 \sin(x) - 1.02 \cos(x),$$

Figure 4



which is shown in Figure 4 as the magenta curve.

UCES

"Overdetermined Systems and Curve Fitting to Data"

Course: Methods and Analysis in UCES

Chapter: 1.0 Matrix Computations

Section: 1.8 Overdetermined Systems and Curve Fitting to Data

Introduction: overdetermined system

Applied Area: business forecasting, nonlinear heat diffusion

Model: least squares

Method: normal equations

Implementation: Maple, Matlab

Assessment: ill-conditioned normal equation

Homework:

Prerequisites:

1. **Math:** Algebra and matrices
2. **Computing:** Maple or Matlab
3. **Science:** Physics

Objectives:

1. **Math:** Minimization, normal equation
2. **Computing:** Overdetermined systems
3. **Science:** Nonlinear thermal properties

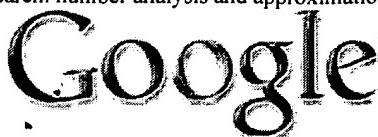
General Information: This is an introduction to curve fitting and to nonlinear aspects of heat transfer. The normal equations are introduced to solve the least squares problem, and the possibility of ill-conditioned normal equations is introduced.

Contact Person: R. E. White, NCSU, white@math.ncsu.edu

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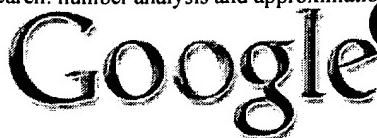
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